

Pentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]non-4-ene: Synthesis, Reactivity, Matrix Isolation Spectroscopy, Calculations, and Physical Study of Reaction Products



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Pyramidalized alkenes are molecules containing carbon–carbon double bonds in which one or both of the doubly bonded carbon atoms do not lie in the plane defined by the three atoms attached to it. My research group is investigating the synthesis and study of pentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]non-4-ene (**2**) (below), a highly pyramidalized alkene. We have shown that dehalogenation of 4,5-diiodopentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]nonane (**1**) with alkyllithiums leads to the title compound **2**, which may be trapped as its Diels-Alder adduct with reactive dienes. However, several alkyllithium addition products, including structures **3**, **4**, and **5**, always accompany the trapped products. Because of the propensity of pentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]non-4-ene (**2**) to react with alkyllithiums present in the reaction mixture, we have been investigating alternative synthetic routes to this molecule. We have made progress toward the synthesis of 4-Iodo-5-(trimethylsilyl)pentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]nonane, and we expect it to act as a precursor to **2** via treatment with fluoride ion. Finally, we have also investigated the reaction of 4,5-diiodopentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]nonane (**1**) with sodium metal in refluxing 1,4-dioxane. This reaction furnishes a mixture of four main products of which three have been conclusively identified as **6**, **8**, and **9**. The fourth product in the mixture has been tentatively identified as **7**.

